

Loop quantum $f(\mathcal{R})$ theories

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As modified gravity theories, the 4-dimensional metric $f(\mathcal{R})$ theories are cast into connection dynamical formalism with real $su(2)$ -connections as configuration variables. This formalism enables us to extend the non-perturbative loop quantization scheme of general relativity to any metric $f(\mathcal{R})$ theories. The quantum kinematical framework of $f(\mathcal{R})$ gravity is rigorously constructed, where the quantum dynamics can be launched. Both Hamiltonian constraint operator and master constraint operator for $f(\mathcal{R})$ theories are well defined. Our results show that the non-perturbative quantization procedure of loop quantum gravity are valid not only for general relativity but also for a rather general class of 4-dimensional metric theories of gravity.

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I. INTRODUCTION

The theoretical search for a quantum theory of gravity has been rather active. Especially, as a background independent approach to quantize general relativity (GR), loop quantum gravity (LQG), has been widely investigated in recent twenty-five years. For reviews in this field, we refer to [1–4]. It is remarkable that, as a non-renormalizable theory, GR can be non-perturbatively quantized by the loop quantization procedure [5]. This background-independent quantization relies on the key observation that classical GR can be cast into the connection dynamical formalism with structure group of $SU(2)$. Thus one is naturally led to ask whether GR is a unique relativistic theory of gravity with connection dynamical character. Recently modified gravity theories have received increased attention in issues related to “dark energy” and non-trivial tests on gravity beyond GR. A series of independent observations, including type Ia supernova, weak lens, cosmic microwave background anisotropy, baryon oscillation, etc, implied that our universe is currently undergoing a period of accelerated expansion [6]. This result conflicts with the prediction of GR and has carried the “dark energy” problem. Although the acceleration could be explained by introducing a cosmological constant Λ , the observed value of Λ is unnaturally much smaller than any estimation by tens of orders. Hence it is reasonable to consider the possibility that GR is not a valid theory of gravity on a cosmological scale. Since it was found that a small modification of the Einstein-Hilbert action by adding an inverse power term of curvature scalar \mathcal{R} would lead to current acceleration of our universe, a large variety of models of $f(\mathcal{R})$ modified gravity have been proposed [7]. Moreover, some models of $f(\mathcal{R})$ gravity may account for the “dark matter” problem, which was revealed by the observed rotation curve of galaxy clusters. We refer to [7, 8] for a recent review on $f(\mathcal{R})$ theories of gravity and its application to cosmology. It is also worth noting that certain effective equation of loop quantum cosmology can be derived from some classical $f(\mathcal{R})$ theory [9].

Historically, Einstein’s GR is the simplest relativistic theory of gravity with correct Newtonian limit. It is worth pursuing all alternatives, which provide a high chance to new physics. Recall that the precession of Mercury’s orbit was at first attributed to some unobserved planet orbiting inside Mercury’s orbit, but was actually explained only after the passage from Newtonian gravity to GR. Given the strong motivation to $f(\mathcal{R})$ gravity, it is desirable to study such kind of theories at fundamental quantum level. For metric $f(\mathcal{R})$ theories, gravity is still geometry as in GR. The differences between them are just reflected in dynamical equations. Hence, a background-independent and non-perturbative quantization for $f(\mathcal{R})$ gravity is preferable. The framework of extending LQG to $f(\mathcal{R})$ theories appeared in [10]. The purpose of this paper is to provide the detailed constructions.

We will show that the connection dynamical formulation of $f(\mathcal{R})$ gravity can be derived by canonical transformations from its geometrical dynamics. The latter was realized by introducing a non-minimally coupled scalar field to replace the original $f(\mathcal{R})$ action and doing Hamiltonian analysis. While the equivalence by canonical transformations at the classical level does not imply equivalence after quantization, our choice of the canonical formalism enables us to carry out the physical and mathematical ideas of LQG. The canonical variables of our Hamiltonian formalism of $f(\mathcal{R})$ gravity consist of $su(2)$ -connection A_a^i and its conjugate momentum E_i^a , as well as the scalar field ϕ and its momentum π . The Gaussian, diffeomorphism and Hamiltonian constraints are also obtained, and they comprise a first-class system. Loop quantization procedure is then naturally employed to quantize $f(\mathcal{R})$ gravity. The rigorous Kinematical Hilbert space structure of loop quantum GR is extended to loop quantum $f(\mathcal{R})$ gravity by adding a polymer-like quantum scalar field. The spatial geometric operators of LQG, such as the area and volume operators are still valid here. Hence the important physical result that both the area and the volume are discrete at quantum kinematical level is also true for $f(\mathcal{R})$ gravity. As in LQG, the Gaussian and diffeomorphism constraints can be solved at quantum level, and both the Hamiltonian constraint and the master constraint can be promoted to well-defined operators.

This paper is organized as follows. In section II, we derive the connection dynamical formalism for $f(\mathcal{R})$ theories. In section III, the kinematical Hilbert space for $f(\mathcal{R})$ gravity is con-

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structed, where the Gaussian and diffeomorphism constraints are implemented. The Hamiltonian constraint is promoted to a well-defined operator in the kinematical Hilbert space in section IV. We also define a self-adjoint master constraint operator in the diffeomorphism invariant Hilbert space in section V. Finally, some concluding remarks are given in section VI. We use Greek alphabet for spacetime indices. Latin alphabet a, b, c, \dots for spatial indices, and i, j, k, \dots for internal indices.

II. CONNECTION DYNAMICAL FORMALISM FOR $f(R)$ THEORY

A simple extension of GR is to consider the Lagrangian of gravity as a function of scalar curvature \mathcal{R} . This kind of modified gravity theories have become topical in cosmology and astro-physics. The original action of $f(\mathcal{R})$ theories read:

$$S(g) = \frac{1}{2} \int d^4x \sqrt{-g} f(\mathcal{R}) \quad (1)$$

where f is a general function of \mathcal{R} , and we set $8\pi G = 1$. By introducing an independent variable s and a Lagrange multiplier ϕ , an equivalent action is proposed as [11, 12]:

$$S(g, \phi, s) = \frac{1}{2} \int d^4x \sqrt{-g} (f(s) - \phi(s - \mathcal{R})). \quad (2)$$

The variation of (2) with respect to s yields

$$\phi = \frac{df(s)}{ds} \equiv f'(s). \quad (3)$$

Assuming $f''(s) \neq 0$ so that s could be resolved from the above equation, action (2) is reduced to

$$S(g, \phi) = \frac{1}{2} \int d^4x \sqrt{-g} (\phi \mathcal{R} - \xi(\phi)) \equiv \int d^4x \mathcal{L}(x) \quad (4)$$

where $\xi(\phi) \equiv \phi s - f(s)$. The variations of (4) give the following equations of motion

$$\phi G_{\mu\nu} = -\frac{1}{2} g_{\mu\nu} \xi(\phi) + \nabla_\mu \nabla_\nu \phi - g_{\mu\nu} \nabla_\sigma \nabla^\sigma \phi, \quad (5)$$

$$\mathcal{R} = \xi'(\phi) \quad (6)$$

where $\xi'(\phi) \equiv \frac{d\xi(\phi)}{d\phi}$, and ∇_μ is the connection compatible with $g_{\mu\nu}$. It is easy to see that Eqs. (5) and (6) are equivalent to the equations of motion derived from action (1). The virtue of action (4) is that it admit a treatable Hamiltonian analysis [11]. The Hamiltonian formalism can be derived by doing 3+1 decomposition and Legendre transformation:

$$\begin{aligned} p^{ab} &= \frac{\partial \mathcal{L}}{\partial \dot{h}_{ab}} \\ &= \frac{\sqrt{h}}{2} [\phi (K^{ab} - K h^{ab}) - \frac{h^{ab}}{N} (\dot{\phi} - N^c \partial_c \phi)], \end{aligned} \quad (7)$$

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = -\sqrt{h} K \quad (8)$$

where h_{ab} and K_{ab} are respectively the induced 3-metric and the extrinsic curvature of the spatial hypersurface Σ and $K \equiv K^a_a$. The combination of the trace of Eq.(7) and Eq.(8) yields

$$\dot{\phi} - N^c \partial_c \phi = \frac{2N}{3\sqrt{h}} (\phi \pi - p). \quad (9)$$

Note that the action (4) is also meaningful for a constant ϕ . In this special case, one could resolve π from p by Eq.(9) as $\pi = p/\phi$. This reduces one degree of freedom of the theory. Then the $f(\mathcal{R})$ theory will be reduced back to GR. In general case, the Hamiltonian of $f(\mathcal{R})$ gravity can be derived as a liner combination of constraints as

$$H_{total} = \int_\Sigma d^3x (N^a V_a + NH). \quad (10)$$

where N and N^a are the lapse function and shift vector respectively, and the smeared diffeomorphism and Hamiltonian constraints read

$$\begin{aligned} V(\vec{N}) &\equiv \int_\Sigma d^3x N^a V_a \\ &= \int_\Sigma d^3x N^a (-2D^b(p_{ab}) + \pi \partial_a \phi), \end{aligned} \quad (11)$$

$$\begin{aligned} H(N) &\equiv \int_\Sigma d^3x NH \\ &= \int_\Sigma d^3x N \left[\frac{2}{\sqrt{h}} \left(\frac{p_{ab} p^{ab} - \frac{1}{3} p^2}{\phi} + \frac{1}{6} \phi \pi^2 - \frac{1}{3} p \pi \right) \right. \\ &\quad \left. + \frac{1}{2} \sqrt{h} (\xi(\phi) - \phi \mathcal{R} + 2D_a D^a \phi) \right], \end{aligned} \quad (12)$$

where D_a is the connection compatible with the 3-metric h_{ab} . Again, in the special case of $\phi = \text{constant}$, it is easy to see that the smeared diffeomorphism and Hamiltonian constraints can go back to GR up to a constant rescale. By the symplectic structure

$$\begin{aligned} \{h_{ab}(x), p^{cd}(y)\} &= \delta_a^c \delta_b^d \delta^3(x, y), \\ \{\phi(x), \pi(y)\} &= \delta^3(x, y), \end{aligned} \quad (13)$$

lengthy but straightforward calculations show that the constraints (11) and (12) comprise a first class system similar to GR as:

$$\begin{aligned} \{V(\vec{N}), V(\vec{N}')\} &= V([\vec{N}, \vec{N}']), \\ \{V(\vec{N}), H(M)\} &= H(\mathcal{L}_{\vec{N}} M), \\ \{H(N), H(M)\} &= V(ND^a M - MD^a N). \end{aligned} \quad (14)$$

Since the above Hamiltonian analysis is started with the action (4) where a non-minimally coupled scalar field is introduced, we need to check whether the Hamiltonian formalism is equivalent to the Lagrangian formalism. It is not difficult to see from the Hamiltonian (10) that the evolution equation of the scalar field reads:

$$\dot{\phi} = \{\phi, H_{total}\} = \frac{2N}{3\sqrt{h}} (\phi \pi - p) + N^a \partial_a \phi \quad (15)$$

which is nothing but the Eq. of (9). The evolution equation of the 3-metric reads

$$\begin{aligned}\dot{h}_{ab} &= \frac{N}{\sqrt{h}} \left(\frac{4(p_{ab} - \frac{1}{3}ph_{ab})}{\phi} - \frac{2}{3}\pi h_{ab} \right) + D_a N_b + D_b N_a \\ &= 2NK_{ab} + D_a N_b + D_b N_a,\end{aligned}\quad (16)$$

which is nothing but the definition of K_{ab} . The evolution equation of the momentum of ϕ reads

$$\begin{aligned}\dot{\pi} &= \partial_a(N^a\pi) + \frac{2N}{\sqrt{h}} \left(\frac{p_{ab}p^{ab} - \frac{1}{3}p^2}{\phi^2} - \frac{1}{6}\pi^2 \right) - \frac{N\sqrt{h}}{2}\xi'(\phi) \\ &+ \frac{N\sqrt{h}}{2}R - \sqrt{h}D_a D^a N \\ &= \partial_a(N^a\pi) + \frac{N\sqrt{h}}{2}(K_{ab}K^{ab} - K^2) - \frac{N\sqrt{h}}{2}\xi'(\phi) \\ &+ \frac{N\sqrt{h}}{2}R - \partial_a(\sqrt{h}h^{ab}\partial_b N).\end{aligned}\quad (17)$$

Using the definition of $\pi = -\sqrt{h}K$ and $n^0 = \frac{1}{N}$, $n^i = -\frac{N^i}{N}$, we can get

$$\begin{aligned}\xi'(\phi) &= K_{ab}K^{ab} - K^2 + R + \frac{2}{N\sqrt{h}}\partial_\nu(\sqrt{-g}n^\nu K) \\ &- \frac{2}{N\sqrt{h}}\partial_a(\sqrt{h}h^{ab}\partial_b N) = \mathcal{R}.\end{aligned}\quad (18)$$

This is nothing but Eq. (6). On the other hand, the 00-component of Eq.(5) reads

$$\phi G_{\mu\nu}n^\mu n^\nu = \frac{\phi}{2}(R - K_{ab}K^{ab} + K^2).\quad (19)$$

Using the identity $g_{\mu\nu}n^\mu n^\nu = -1$, Eq.(19) becomes

$$\begin{aligned}&\frac{\phi}{2}(R - K_{ab}K^{ab} + K^2) \\ &= \frac{1}{2}\xi(\phi) + (g^{\mu\nu} + n^\mu n^\nu)\nabla_\mu \nabla_\nu \phi \\ &= \frac{1}{2}\xi(\phi) + D_a D^a \phi - K\left(\frac{1}{N}(\dot{\phi} - N^c \partial_c \phi)\right)\end{aligned}\quad (20)$$

where the facts $h^{\mu\nu}n_\nu = 0$ and $n^\sigma \partial_\sigma \phi = \frac{1}{N}(\dot{\phi} - N^c \partial_c \phi)$ have been used in the above derivation. Note that the Hamiltonian constraint in Eq.(12) can be expressed as

$$\begin{aligned}H &= \frac{\sqrt{h}\phi}{2}(K_{ab}K^{ab} - K^2 - R) + \frac{\sqrt{h}}{2}(\xi(\phi) + 2D_a D^a \phi) \\ &- \sqrt{h}K\left(\frac{1}{N}(\dot{\phi} - N^c \partial_c \phi)\right).\end{aligned}\quad (21)$$

Hence the 00-component of (5) is equivalent to Hamiltonian constraint. Now we come to the 0a-component of (5). Since

$$\phi G_{\mu\nu}n^\mu h_a^\nu = \phi(D_a K_a^a - D_a K) \quad \text{and} \quad g_{\mu\nu}n^\mu h_a^\nu = 0,\quad (22)$$

we have

$$\begin{aligned}\phi(D_a K_b^a - D_b K) &= n^\nu h_b^\sigma \nabla_\sigma \nabla_\nu \phi \\ &= n^\nu h_b^\sigma \nabla_\sigma ((h_\nu^\mu - n^\mu n_\nu)\partial_\mu \phi).\end{aligned}\quad (23)$$

The first term in the right hand side of above equation reads

$$\begin{aligned}n^\nu h_a^\sigma \nabla_\sigma (h_\nu^\mu \partial_\mu \phi) &= n^\nu h_a^\sigma \nabla_\sigma (g_\nu^\mu + n^\mu n_\nu)\partial_\mu \phi \\ &= -K_a^b \partial_b \phi,\end{aligned}\quad (24)$$

and the second term reads

$$\begin{aligned}-n^\nu h_a^\sigma \nabla_\sigma (n^\mu n_\nu \partial_\mu \phi) &= h_a^\sigma \nabla_\sigma (n^\mu \partial_\mu \phi) \\ &= D_a \left(\frac{1}{N}(\dot{\phi} - N^c \partial_c \phi) \right).\end{aligned}\quad (25)$$

Hence their combination gives

$$\begin{aligned}&D_a(\phi K_b^a) - D_b(\phi K) + K D_b \phi - D_b \left(\frac{1}{N}(\dot{\phi} - N^c \partial_c \phi) \right) \\ &= \frac{2}{\sqrt{h}} D_a \left(\frac{\sqrt{h}}{2} [\phi(K_b^a - K h_b^a) - \frac{h_b^a}{N}(\dot{\phi} - N^c \partial_c \phi)] \right) \\ &- \frac{\pi}{\sqrt{h}} \partial_b \phi.\end{aligned}\quad (26)$$

This is nothing but the diffeomorphism constraint in Eq.(11). Now we turn to the ab-components of (5). We will show that they are equivalent to the equation of motion of p_{ab} which reads

$$\begin{aligned}\dot{p}_{ab} &= \frac{h_{ab}N}{\sqrt{h}} \left(\frac{p_{cd}p^{cd} - \frac{1}{3}p^2}{\phi} + \frac{1}{6}\phi\pi^2 - \frac{1}{3}p\pi \right) \\ &+ \frac{2N}{\sqrt{h}} \left(\frac{p_{ac}p_b^c - \frac{1}{3}pp_{ab}}{\phi} - \frac{1}{3}p_{ab}\pi \right) \\ &+ \frac{N}{4}\sqrt{h}h_{ab}\phi R - \frac{N}{2}\sqrt{h}\phi R_{ab} - \frac{N}{4}\sqrt{h}h_{ab}\xi(\phi) \\ &- \frac{N}{2}\sqrt{h}h_{ab}D_c D^c \phi - D_{(a}N\sqrt{h}D_{b)}\phi \\ &+ \frac{\sqrt{h}}{2}(D_{(a}D_{b)}(N\phi) - h_{ab}D_c D^c(N\phi)) \\ &+ 2p_{c(a}D^{cN_{b)} + D_c(p_{ab}N^c).\end{aligned}\quad (27)$$

Since the initial value formalism of $f(\mathcal{R})$ theories has been obtained in [7], we will use Eq.(27) to derive the time derivative of the extrinsic curvature:

$$K_{ab} = \frac{2(p_{ab} - \frac{1}{3}ph_{ab})}{\phi\sqrt{h}} - \frac{\pi h_{ab}}{3\sqrt{h}}.\quad (28)$$

A straightforward calculation yields

$$\begin{aligned}\dot{K}_{ab} &= 2NK_{ac}K_b^c - NKK_{ab} + \mathcal{L}_{\vec{N}}K_{ab} - NR_{ab} \\ &+ D_a D_b N + \frac{N}{\phi}D_a D_b \phi \\ &+ \frac{Nh_{ab}}{6}(\xi'(\phi) + \frac{\xi(\phi)}{\phi}) - \frac{n^\sigma \partial_\sigma \phi}{\phi}NK_{ab}.\end{aligned}\quad (29)$$

It is easy to see that Eq.(29) is equivalent to Eq.(217) in [7]. Note that there is a sign difference between the definition of our extrinsic curvature and that in [7], and our potential $\xi(\phi)$ is twice of that in [7]. To summarize, we have shown that the Hamiltonian formalism of $f(\mathcal{R})$ gravity is equivalent to its Lagrangian formalism.

Recall that the non-perturbative loop quantization of GR was based on its connection dynamic formalism. It is very interesting to study whether the previous geometric dynamics of $f(\mathcal{R})$ modified gravity also has a connection dynamic correspondence. To this aim, we first extend the phase space of geometrical dynamics to the triad formalism, and then introduce a canonical transformation on the extended phase space of $f(\mathcal{R})$ theories. Let

$$\begin{aligned}\tilde{K}^{ab} &\equiv \phi K^{ab} + \frac{h^{ab}}{2N}(\dot{\phi} - N^c \partial_c \phi) \\ &= \phi K^{ab} + \frac{h^{ab}}{3\sqrt{h}}(\phi\pi - p),\end{aligned}\quad (30)$$

and $E_i^a \equiv \sqrt{h}e_i^a$, where e_i^a is the triad s.t. $h_{ab}e_i^a e_j^b = \delta_{ij}$. Then we get

$$\begin{aligned}p^{ab} &= \frac{\sqrt{h}}{2}(\tilde{K}^{ab} - \tilde{K}_c^{ab}h^{ab}) \\ &= \frac{1}{2}(\tilde{K}_i^a E^{bi} - \frac{1}{h}\tilde{K}_c^i E^c E_j^b E_j^b), \\ \pi &= -\frac{\sqrt{h}}{\phi}(\tilde{K}_c^c - \frac{3}{2N}(\dot{\phi} - N^c \partial_c \phi)),\end{aligned}\quad (31)$$

where $\tilde{K}_i^a \equiv \tilde{K}^{ab}e_b^i$. Now we extend the phase space of geometry to the space consisting of pairs (E_i^a, \tilde{K}_i^a) . It is then easy to see that the symplectic structure (13) can be derived from the following Poisson brackets:

$$\begin{aligned}\{E_j^a(x), E_k^b(y)\} &= \{\tilde{K}_a^j(x), \tilde{K}_b^k(y)\} = 0, \\ \{\tilde{K}_a^j(x), E_k^b(y)\} &= \delta_a^b \delta_k^j \delta(x, y).\end{aligned}\quad (32)$$

Thus there is a symplectic reduction from the extended phase space to the original one, and the transformation from conjugate pairs (h_{ab}, p^{cd}) to (E_i^a, \tilde{K}_i^a) is "canonical" in this sense. Note that since $\tilde{K}^{ab} = \tilde{K}^{ba}$, we have an additional constraint:

$$G_{jk} \equiv \tilde{K}_{a[j} E_{k]}^a = 0. \quad (33)$$

So we can further make a canonical transformation by defining:

$$A_a^i = \Gamma_a^i + \gamma \tilde{K}_a^i. \quad (34)$$

where Γ_a^i is the spin connection determined by E_i^a , and γ is a nonzero real number. It is clear that our new variable A_a^i coincides with the Ashtekar-Barbero connection [13, 14] when $\phi = 1$. The Poisson brackets among the new variables read:

$$\begin{aligned}\{A_a^i(x), E_b^j(y)\} &= \gamma \delta_a^b \delta_k^j \delta(x, y), \\ \{A_a^i(x), A_b^j(y)\} &= 0.\end{aligned}\quad (35)$$

Now, the phase space of $f(\mathcal{R})$ gravity consists of conjugate pairs (A_a^i, E_b^j) and (ϕ, π) . Combining Eq.(33) with the compatibility condition:

$$\partial_a E_i^a + \epsilon_{ijk} \Gamma_a^j E^a = 0, \quad (36)$$

we obtain the standard Gaussian constraint

$$\mathcal{G}_i = \mathcal{D}_a E_i^a \equiv \partial_a E_i^a + \epsilon_{ijk} A_a^j E^a \quad (37)$$

which justifies A_a^i as an $su(2)$ -connection. Note that, had we let $\gamma = \pm i$, the (anti-)self-dual complex connection formalism would be obtained. The original diffeomorphism constraint can be expressed in terms of new variables up to Gaussian constraint as

$$\begin{aligned}V_a &= -2D^b(p_{ab}) + \pi \partial_a \phi \\ &= \frac{1}{\gamma} F_{ab}^i E_i^b + \pi \partial_a \phi,\end{aligned}\quad (38)$$

where $F_{ab}^i \equiv 2\partial_{[a} A_{b]}^i + \epsilon_{kl}^i A_a^k A_b^l$ is the curvature of A_a^i . The original Hamiltonian constraint can be written up to Gaussian constraint as

$$\begin{aligned}H &= \frac{\phi}{2} [F_{ab}^j - (\gamma^2 + \frac{1}{\phi^2}) \epsilon_{jmn} \tilde{K}_a^m \tilde{K}_b^n] \frac{\epsilon_{jkl} E_k^a E_l^b}{\sqrt{h}} \\ &+ \frac{1}{2} \left(\frac{2}{3\phi} \frac{(\tilde{K}_a^i E_i^a)^2}{\sqrt{h}} + \frac{4}{3} \frac{(\tilde{K}_a^i E_i^a) \pi}{\sqrt{h}} + \frac{2}{3} \frac{\pi^2 \phi}{\sqrt{h}} \right) \\ &+ \sqrt{h} \xi(\phi) + \sqrt{h} D_a D^a \phi.\end{aligned}\quad (39)$$

It is easy to check that the smeared Gaussian constraint, $\mathcal{G}(\Lambda) := \int_{\Sigma} d^3x \Lambda^i(x) \mathcal{G}_i(x)$, generates $SU(2)$ gauge transformations on the phase space, while the smeared constraint

$$\mathcal{V}(\vec{N}) := \int_{\Sigma} d^3x N^a (V_a - A_a^i \mathcal{G}_i) \quad (40)$$

generates spatial diffeomorphism transformations on the phase space. Together with the smeared Hamiltonian constraint $H(N) = \int_{\Sigma} d^3x N H$, we can show that the constraints algebra has the following form:

$$\{\mathcal{G}(\Lambda), \mathcal{G}(\Lambda')\} = \mathcal{G}([\Lambda, \Lambda']), \quad (41)$$

$$\{\mathcal{G}(\Lambda), \mathcal{V}(\vec{N})\} = -\mathcal{G}(\mathcal{L}_{\vec{N}} \Lambda), \quad (42)$$

$$\{\mathcal{G}(\Lambda), H(N)\} = 0, \quad (43)$$

$$\{\mathcal{V}(\vec{N}), \mathcal{V}(\vec{N}')\} = \mathcal{V}([\vec{N}, \vec{N}']), \quad (44)$$

$$\{\mathcal{V}(\vec{N}), H(M)\} = H(\mathcal{L}_{\vec{N}} M), \quad (45)$$

$$\begin{aligned}\{H(N), H(M)\} &= \mathcal{V}(ND^a M - MD^a N) \\ &+ \mathcal{G}((N\partial_a M - M\partial_a N)h^{ab}A_b) \\ &- \frac{[E^a D_a N, E^b D_b M]^i}{h} \mathcal{G}_i \\ &- \gamma^2 \frac{[E^a D_a(\phi N), E^b D_b(\phi M)]^i}{h} \mathcal{G}_i.\end{aligned}\quad (46)$$

One may understand Eqs.(41-45) by the geometrical interpretations of $\mathcal{G}(\Lambda)$ and $\mathcal{V}(\vec{N})$. The detail calculation on the Poisson bracket (46) between the two smeared Hamiltonian constraints will be presented in the Appendix. Hence the constraints are of first class. Moreover, the constraint algebra of GR can be recovered for the special case when $\phi = 1$. The

total Hamiltonian is a linear combination of the above constraints as

$$\mathcal{H}_{tot} = \int_{\Sigma} H(N) + N^a V_a + \mathcal{G}(\Lambda). \quad (47)$$

To summarize, $f(\mathcal{R})$ theories of gravity have been cast into the $su(2)$ -connection dynamical formalism. Though a scalar field is non-minimally coupled, the resulted Hamiltonian structure is similar to GR. Note that what we obtain is real $su(2)$ -connection dynamics of Lorentian $f(\mathcal{R})$ gravity rather than the connection dynamics of some conformal theories[15, 16].

III. QUANTUM KINEMATIC OF $f(\mathcal{R})$ THEORY

Recall that LQG is based on the connection dynamics of GR. We have shown in last section that $f(\mathcal{R})$ theories can also be reformulated as connection dynamical theories by introducing a non-minimally coupled scalar field. Hence the non-perturbative loop quantization procedure can be straightforwardly generalized to $f(\mathcal{R})$ theories. Since the configuration space consists of geometry sector and scalar sector, we expect the kinematical Hilbert space of the system to be a direct product of the Hilbert space of geometry and that of scalar field. To construct quantum kinematics for geometry as in LQG, we have to extend the space \mathcal{A} of smooth connections to space $\tilde{\mathcal{A}}$ of distributional connections. A simple element $\bar{A} \in \tilde{\mathcal{A}}$ may be thought as a holonomy,

$$h_e(A) = \mathcal{P} \exp \int_e A_a \quad (48)$$

of a connection along an edge $e \subset \Sigma$. Through projective techniques, $\tilde{\mathcal{A}}$ is equipped with a natural measure μ_0 , called the Ashtekar-Lewandowski measure[3, 4]. On the other hand, one may smear the densitized triad E_i^a on 2-surfaces to obtain fluxes as

$$E(S, f) := \int_S \epsilon_{abc} E_i^a f^i \quad (49)$$

where f^i is a $su(2)$ -valued function on S . From the algebraic viewpoint, the cylindrical functions of holonomies and the fluxes consist of an C^* -algebra. Then by Gel'fand-Naimark-Segal(GNS) structure[2], one can obtain the cyclic representation for the quantum holonomy-flux $*$ -algebra, which coincides with the one by projective techniques. In a certain sense, this is the unique diffeomorphism and internal gauge invariant representation for the quantum holonomy-flux algebra[17]. The kinematical Hilbert space of geometry then reads $\mathcal{H}_{kin}^{gr} = L^2(\tilde{\mathcal{A}}, d\mu_0)$. A typical vector $\Psi_{\alpha}(\bar{A}) \in \mathcal{H}_{kin}^{gr}$ is a cylindrical function over some finite graph $\alpha \subset \Sigma$. The so-called spin-network basis

$$T_{\alpha}(\bar{A}) = \prod_{e \in E(\alpha)} \sqrt{2j_e + 1} \pi_{m_e, n_e}^{j_e}(\bar{A}(e)), \quad (j_e \neq 0) \quad (50)$$

provides an orthonormal basis for \mathcal{H}_{kin}^{gr} [3, 4], where $\pi_{m_e, n_e}^{j_e}(\bar{A}(e))$ denotes the matrix elements in the spin- j representation of $SU(2)$. Note that the spatial geometric operator of LQG, such as the area[18], the volume[19] and the length[20, 21] operators, are still valid in \mathcal{H}_{kin}^{gr} , though their properties in the physical Hilbert space still need to be clarified [22, 23].

Since the scalar field also reflects $f(\mathcal{R})$ gravity, it is natural to employ the polymer-like representation for its quantization [24]. In this representation, one extends the space \mathcal{U} of smooth scalar fields to the quantum configuration space $\tilde{\mathcal{U}}$. A simple element $\bar{U} \in \tilde{\mathcal{U}}$ may be thought as a point holonomy,

$$U_{\lambda} = \exp(i\lambda\phi(x)), \quad (51)$$

at point $x \in \Sigma$, where λ is a real number. By GNS structure[2], there is a natural diffeomorphism invariant measure $d\mu$ on $\tilde{\mathcal{U}}$ [24]. Thus the kinematical Hilbert space of scalar field reads $\mathcal{H}_{kin}^{sc} = L^2(\tilde{\mathcal{U}}, d\mu)$. The following scalar-network function of ϕ :

$$T_X(\phi) \equiv T_{X, \lambda}(\phi) = \prod_{x_j \in X} U_{\lambda}(\phi(x_j)), \quad (52)$$

where $X = \{x_1, \dots, x_n\}$ is an arbitrary given set of finite number of points in Σ , constitute a complete set of orthonormal basis in \mathcal{H}_{kin}^{sc} . Since the point holonomy of a scalar is defined on an 0-dimensional point, the momentum is smeared on a 3-dimensional region R in Σ as:

$$\pi(R) := \int_R d^3x \pi(x). \quad (53)$$

Thus the total kinematical Hilbert space for $f(\mathcal{R})$ gravity reads $\mathcal{H}_{kin} := \mathcal{H}_{kin}^{gr} \otimes \mathcal{H}_{kin}^{sc}$ with an orthonormal basis $T_{\alpha, X}(A, \phi) \equiv T_{\alpha}(A) \otimes T_X(\phi)$. Note that a basic feature of loop quantization is that only holonomies will become configuration operators, rather than the classical configuration variables themselves. Let $\Psi(A, \phi)$ denote a quantum state in \mathcal{H}_{kin} . The actions of basic operators read

$$\begin{aligned} \hat{h}_e(A)\Psi(A, \phi) &= h_e(A)\Psi(A, \phi), \\ \hat{E}(S, f)\Psi(A, \phi) &= i\hbar\{E(S, f), \Psi(A, \phi)\}, \\ \hat{U}_{\lambda}(\phi(v))\Psi(A, \phi) &= \exp(i\lambda\phi(v))\Psi(A, \phi), \\ \hat{\pi}(R)\Psi(A, \phi) &= i\hbar\{\pi(R), \Psi(A, \phi)\}. \end{aligned} \quad (54)$$

As in LQG, it is straight-forward to promote the Gaussian constraint $\mathcal{G}(\Lambda)$ to a well-defined operator in \mathcal{H}_{kin} . It's kernel is the internal gauge invariant Hilbert space \mathcal{H}_G with gauge invariant spin-scalar-network basis $T_{s,c} = T_s(A) \otimes T_X(\phi)$, where

$$T_{s=(\alpha, j, i)}(A) = \otimes_{v \in V(\alpha)} i_v \cdot \otimes \pi^{j_e}(\bar{A}(e)), \quad (j_e \neq 0). \quad (55)$$

Here an intertwiner i is assigned to each vertex of graph α . All the internal gauge invariant geometric operators, such as the area, volume and length, can also be well defined in \mathcal{H}_G . Since the diffeomorphisms of Σ act covariantly on the cylindrical functions in \mathcal{H}_G , the so-called group averaging technique can be employed to solve the diffeomorphism constraint[3, 4]. To

this aim, we first define a projection map acting on cylindrical functions $\psi_\beta \equiv \psi_{\alpha, X}(A, \phi) \in \mathcal{H}_{\text{kin}}$ as

$$\hat{P}_{\text{Diff}_\beta} \psi_\beta := \frac{1}{n_\beta} \sum_{\varphi \in GS_\beta} \hat{U}_\varphi \psi_\beta, \quad (56)$$

where \hat{U}_φ denotes the unitary operator corresponding to a finite diffeomorphism $\varphi : \Sigma \rightarrow \Sigma$. Here $GS_\beta = \text{Diff}_\beta / T\text{Diff}_\beta$ is the group of graph symmetries, where Diff_β is the group of all diffeomorphisms preserving the colored β , $T\text{Diff}_\beta$ is the group of diffeomorphisms which trivially acts on β , and n_β is the number of the elements in GS_β . Secondly, we average with respect to all remaining diffeomorphisms which change the graph β . For each cylindrical function ψ_β , there is an element $\eta(\psi_\beta)$ associated to it in the algebraic dual space Cyl^* which acts on any cylindrical function $\phi_{\beta'}$ as

$$\eta(\psi_\beta)[\phi_{\beta'}] := \sum_{\varphi \in \text{Diff}(\Sigma)/\text{Diff}_\beta} \langle \hat{U}_\varphi \hat{P}_{\text{Diff}_\beta} \psi_\beta | \phi_{\beta'} \rangle_{\text{kin}}, \quad (57)$$

where $\text{Diff}(\Sigma)$ is the diffeomorphism group of Σ . It is easy to verify that $\eta(\psi_\beta)$ is invariant under the group action of $\text{Diff}(\Sigma)$, since

$$\eta(\psi_\beta)[\hat{U}_\varphi \phi_{\beta'}] = \eta(\psi_\beta)[\phi_{\beta'}]. \quad (58)$$

Thus we have defined a rigging map $\eta : \text{Cyl} \rightarrow \text{Cyl}^*_{\text{Diff}}$, which maps every cylindrical function to a diffeomorphism invariant one. Moreover, a Hermitian inner product can be defined on $\text{Cyl}^*_{\text{Diff}}$ via the natural action of the algebraic functional:

$$\langle \eta(\psi_\beta) | \eta(\phi_{\beta'}) \rangle_{\text{Diff}} := \eta(\psi_\beta)[\phi_{\beta'}]. \quad (59)$$

The diffeomorphism invariant Hilbert space $\mathcal{H}_{\text{Diff}}$ is defined by the completion of $\text{Cyl}^*_{\text{Diff}}$ with respect to the above inner product. Thus we can also obtain the desired diffeomorphism and gauge invariant Hilbert space, $\mathcal{H}_{\text{Diff}}$, for $f(\mathcal{R})$ gravity.

IV. QUANTUM HAMILTONIAN OF $f(\mathcal{R})$ THEORY

While the kinematical frameworks of LQG and polymer-like scalar field have been straight-forwardly extended to $f(\mathcal{R})$ theories, the nontrivial task is to implement the Hamiltonian constraint (39) at quantum level. In this section, we can show by detail and technical analysis that, as in LQG, the Hamiltonian constraint can be promoted to a well-defined operator in the kinematical Hilbert space \mathcal{H}_{kin} . The resulted Hamiltonian constraint operator is internal gauge invariant and diffeomorphism covariant. Hence it is at least well defined in the gauge invariant Hilbert space \mathcal{H}_G .

Comparing Eq.(39) with the Hamiltonian constraint of GR in connection formalism, the new ingredient of $f(\mathcal{R})$ gravity that we have to deal with are $\phi(x)$, $\phi^{-1}(x)$, $\xi(\phi)$ and the following four terms

$$\begin{aligned} H_3 &= \int_\Sigma d^3x \frac{N}{3\phi} \frac{(\tilde{K}_a^i E_i^a)^2}{\sqrt{h}}, \\ H_4 &= \int_\Sigma d^3x \frac{2N}{3} \frac{(\tilde{K}_a^i E_i^a) \pi}{\sqrt{h}}, \\ H_5 &= \int_\Sigma d^3x \frac{N}{3} \frac{\pi^2 \phi}{\sqrt{h}}, \\ H_7 &= \int_\Sigma d^3x N \sqrt{h} D_a D^a \phi. \end{aligned} \quad (60)$$

Here we have written the smeared version of Eq.(39) as $H(N) = \sum_{i=1}^7 H_i$. Note that the first two terms in $H(N)$ can be written as

$$\begin{aligned} H_1 &= \frac{1}{2} \int_\Sigma d^3x N \phi F_{ab}^j \frac{\varepsilon_{jkl} E_k^a E_l^b}{\sqrt{h}} \\ &= H^{\text{Eucl}}(\phi N), \end{aligned} \quad (61)$$

$$\begin{aligned} H_2 &= -\frac{1}{2} \int_\Sigma d^3x N (\gamma^2 \phi + \frac{1}{\phi}) \varepsilon_{jmn} \tilde{K}_a^m \tilde{K}_b^n \frac{\varepsilon_{jkl} E_k^a E_l^b}{\sqrt{h}} \\ &= \frac{1}{1 + \gamma^2} \mathcal{T}(N(\gamma^2 \phi + \frac{1}{\phi})), \end{aligned} \quad (62)$$

where $\mathcal{T}(N)$ denotes the Lorentzian term in the Hamiltonian constraint of GR. Hence, except that the smearing functions are multiplied by some function of ϕ , these terms keep the same forms as those in GR.

By introducing certain small constant λ_0 , an operator corresponding to the scalar $\phi(x)$ at $x \in \Sigma$ can be defined as

$$\hat{\phi}(x) = \frac{1}{2i\lambda_0} (U_{\lambda_0}(\phi(x)) - U_{-\lambda_0}(\phi(x))). \quad (63)$$

The ambiguity of λ_0 is the price that we have to pay in order to represent field ϕ in the polymer-like representation. To further define an operator corresponding to $\phi^{-1}(x)$, we can use the classical identity

$$\phi^{-1}(x) = \text{sgn}[\phi] (\frac{1}{\text{sgn}[\phi]} |\phi|^l(x), \pi(R))^{1-l}, \quad (64)$$

for any rational number $l \in (0, 1)$, where $\text{sgn}[\phi]$ denotes the sign function of ϕ , $|\phi|$ is the absolute value of ϕ and $x \in R$. For example, one may choose $l = \frac{1}{2}$ for positive $\phi(x)$ and replace the Poisson bracket by commutator to define

$$\hat{\phi}^{-1}(x) = (\frac{2}{i\hbar} [\sqrt{\hat{\phi}(x)}, \hat{\pi}(R)])^2. \quad (65)$$

Thus all the functions $\xi(\phi)$ which can be expanded as powers of $\phi(x)$ have been quantized. For other non-trivial types of $\xi(\phi)$, we may replace the argument ϕ by $\hat{\phi}$ in Eq.(63), provided that no divergence would arise after the replacement. In the case where divergence does appear, there remain the possibilities to employ tricks similar to Eq.(64) to deal with

it. Hence it is reasonable to believe that most physically interesting functions $\xi(\phi)$ can be quantized. Then it is straightforward to quantize $H_6 = \frac{1}{2} \int_{\Sigma} N \sqrt{h} \cdot \xi(\phi)$ as an operator acting on an basis vector $T_{\alpha,X}$ as

$$\hat{H}_6 \cdot T_{\alpha,X} = \frac{1}{2} \sum_{v \in V(\alpha)} N(v) \hat{\xi}(\phi(v)) \hat{V}_v \cdot T_{\alpha,X}. \quad (66)$$

Note that the action of the volume operator \hat{V} on a spin-network basis vector $T_{\alpha}(A)$ over a graph α can be factorized as

$$\hat{V} \cdot T_{\alpha} = \sum_{v \in V(\alpha)} \hat{V}_v \cdot T_{\alpha}. \quad (67)$$

Moreover, by the regularization techniques developed for the Hamiltonian constraint operators of LQG and polymer-like scalar field, all the terms H_3, H_4, H_5 and H_7 can be regularized as operators acting on cylindrical functions in \mathcal{H}_{kin} in state-dependent ways. In the regularization procedure, we will use the following classical identities

$$\tilde{K}_a^i = \frac{1}{\gamma} \{A_a^i, \tilde{K}\}, \quad (68)$$

where $\tilde{K} = \int_{\Sigma} d^3x \tilde{K}_a^i E_i^a$ can be write as Poisson bracket:

$$\tilde{K} = \gamma^{-\frac{3}{2}} \{H^{\text{Eucl}}(1), V\}. \quad (69)$$

Here the Euclidean scalar constraint $H^{\text{Eucl}}(1)$ by definition was:

$$H^{\text{Eucl}}(1) = \frac{1}{2} \int_{\Sigma} d^3x F_{ab}^j \frac{\varepsilon_{jkl} E_k^a E_l^b}{\sqrt{h}}. \quad (70)$$

Both H^{Eucl} and the volume V under consideration have been quantized in LQG. Also, one has $E_i^a = \frac{1}{2} \varepsilon_{ijk} \epsilon^{abc} e_b^j e_c^k$, where ϵ^{abc} is the levi-civita tensor density, and the co-triad satisfies

$$e_a^i = \frac{2}{\gamma} \{A_a^i(x), V\}. \quad (71)$$

To deal with the four new terms (60), we first regularize them separately by point-splitting and obtain

$$\begin{aligned} H_3 &= \lim_{\epsilon \rightarrow 0} \int_{\Sigma} d^3y \int_{\Sigma} d^3x \frac{N}{3\phi} \chi_{\epsilon}(x-y) \frac{\tilde{K}_a^i(x) E_i^a(x)}{\sqrt{V_{U_x^{\epsilon}}}} \frac{\tilde{K}_b^j(y) E_j^b(y)}{\sqrt{V_{U_x^{\epsilon}}}} \\ &= \lim_{\epsilon \rightarrow 0} \frac{4}{3\gamma^3} \frac{N}{\phi} \chi_{\epsilon}(x-y) \{H^{\text{Eucl}}(1), \sqrt{V_{U_x^{\epsilon}}}\} \\ &\quad \{H^{\text{Eucl}}(1), \sqrt{V_{U_y^{\epsilon}}}\}, \end{aligned} \quad (72)$$

$$\begin{aligned} H_4 &= \lim_{\epsilon \rightarrow 0} \frac{2^{15}}{3^4 \gamma^6} \int_{\Sigma} d^3y \pi(y) \chi_{\epsilon}(w-y) \\ &\quad \times \int_{\Sigma} d^3x N \chi_{\epsilon}(x-y) \{A_a^i(x), \tilde{K}\} \\ &\quad \times \epsilon^{abc} \text{Tr}(\tau_i \{A_b(x), (V_{U_x^{\epsilon}})^{3/4}\} \{A_c(x), (V_{U_x^{\epsilon}})^{3/4}\}) \\ &\quad \times \int_{\Sigma} d^3w \epsilon^{def} \text{Tr}(\{A_d(w), \sqrt{V_{U_w^{\epsilon}}}\} \{A_e(w), \sqrt{V_{U_w^{\epsilon}}}\} \\ &\quad \times \{A_f(w), \sqrt{V_{U_w^{\epsilon}}}\}), \end{aligned} \quad (73)$$

$$\begin{aligned} H_5 &= \lim_{\epsilon \rightarrow 0} \int_{\Sigma} d^3y \int_{\Sigma} d^3x \frac{N\phi}{3} \chi_{\epsilon}(x-y) \pi(x) \pi(y) \\ &\quad \times \int_{\Sigma} d^3u \frac{\det(e_a^i(u))}{(V_{U_u^{\epsilon}}^{\epsilon})^{3/2}} \chi_{\epsilon}(u-x) \\ &\quad \times \int_{\Sigma} d^3w \frac{\det(e_a^i(w))}{(V_{U_w^{\epsilon}}^{\epsilon})^{3/2}} \chi_{\epsilon}(w-y) \\ &= \lim_{\epsilon \rightarrow 0} \frac{2^{14}}{3^3 \gamma^6} \int_{\Sigma} d^3y \int_{\Sigma} d^3x N \phi \pi(x) \pi(y) \\ &\quad \chi_{\epsilon}(x-y) \chi_{\epsilon}(u-x) \chi_{\epsilon}(w-y) \\ &\quad \times \int_{\Sigma} d^3u \epsilon^{abc} \text{Tr}(\{A_a(u), \sqrt{V_{U_u^{\epsilon}}}\} \\ &\quad \{A_b(u), \sqrt{V_{U_u^{\epsilon}}}\} \{A_c(u), \sqrt{V_{U_u^{\epsilon}}}\}) \\ &\quad \times \int_{\Sigma} d^3w \epsilon^{def} \text{Tr}(\{A_d(w), \sqrt{V_{U_w^{\epsilon}}}\} \\ &\quad \{A_e(w), \sqrt{V_{U_w^{\epsilon}}}\} \{A_f(w), \sqrt{V_{U_w^{\epsilon}}}\}), \end{aligned} \quad (74)$$

$$\begin{aligned} H_7 &= - \int_{\Sigma} d^3x D_a (N E_i^a) \frac{1}{\sqrt{h}} E_i^b D_b \phi \\ &= \lim_{\epsilon \rightarrow 0} \int_{\Sigma} d^3y \int_{\Sigma} d^3x (D_a \chi_{\epsilon}(x-y)) \\ &\quad \times N(x) E_i^a(x) \\ &\quad \times (D_b \phi(y)) \frac{E_i^b(y)}{\epsilon^3 (h(y))^{1/2}} \\ &= - \lim_{\epsilon \rightarrow 0} \frac{2^5}{\gamma^2} \int_{\Sigma} d^3y \int_{\Sigma} d^3x (D_a \chi_{\epsilon}(x-y)) N(x) E_i^a(x) \\ &\quad \times \epsilon^{bef} (D_b \phi(y)) \text{Tr}(\tau_i \{A_e(y), (V_{U_y^{\epsilon}})^{1/2}\} \{A_f(y), (V_{U_y^{\epsilon}})^{1/2}\}), \end{aligned} \quad (75)$$

where $\chi_{\epsilon}(x-y)$ is the characteristic function of a box U_x^{ϵ} containing x with scale ϵ and satisfies the relation $\lim_{\epsilon \rightarrow 0} \chi_{\epsilon}(x-y)/\epsilon^3 = \delta(x-y)$, and $V_{U_x^{\epsilon}}$ denote the volume of U_x^{ϵ} . It is easy to see that the regulator in H_3 can be removed by acting on a given basis vector $T_{\alpha,X} \in \mathcal{H}_{\text{kin}}$ as

$$\begin{aligned} \hat{H}_3 \cdot T_{\alpha,X} &= \sum_{v \in V(\alpha)} \frac{4N(v)}{3\gamma^3 (i\hbar)^2} \hat{\phi}^{-1}(v) \\ &\quad \times [H^{\text{Eucl}}(1), \sqrt{\hat{V}_v}] [H^{\text{Eucl}}(1), \sqrt{\hat{V}_v}] \cdot T_{\alpha,X}, \end{aligned} \quad (76)$$

For the other three terms, in order to reexpress connection by holonomy and make the regularization diffeomorphism covariant, we triangulate Σ in adaptation to some graph α underlying a cylindrical function in \mathcal{H}_{kin} . At every vertex $v \in V(\alpha)$, for each triple (e_I, e_J, e_K) of edges of α we have a tetrahedron $\Delta_{\alpha, e_I, e_J, e_K}^{\epsilon}$ based at v , which is spanned by segments s_I, s_J, s_K of the triple. Each segment s_I is given by the part with the curve parameter $t^I \in [0, \epsilon]$ of the corresponding edge $e_I(t^I)$. For each $\Delta_{\alpha, e_I, e_J, e_K}^{\epsilon}$ one can construct seven additional tetrahedron by backward analytic extension of the segments. The regions

of Σ without a vertex of α can be triangulated arbitrarily. Note that for one segment s_I , we have

$$\int_{s_I} \{A(u), \sqrt{V(u, \epsilon)}\} \approx \epsilon \dot{s}_I^a(0) \{A_a(v), \sqrt{V(u, \epsilon)}\} \quad (77)$$

up to $O(\epsilon^2)$. Hence for each $\Delta_{\alpha, v, e_I, e_J, e_K}^\epsilon$, we have

$$\begin{aligned} & \int_{\Delta_{\alpha, v, e_I, e_J, e_K}^\epsilon} \epsilon^{abc} \text{Tr}(\{A_a(u), \sqrt{V_u^\epsilon}\} \{A_b(u), \sqrt{V_u^\epsilon}\} \{A_c(u), \sqrt{V_u^\epsilon}\}) \\ & \approx -\frac{1}{6} \epsilon(s_I s_J s_K) \epsilon^{IJK} \text{Tr}(h_{s_I(\Delta)} \{h_{s_I(\Delta)}^{-1}, \sqrt{V_{v(\Delta)}^\epsilon}\} \\ & \times h_{s_J(\Delta)} \{h_{s_J(\Delta)}^{-1}, \sqrt{V_{v(\Delta)}^\epsilon}\} h_{s_K(\Delta)} \{h_{s_K(\Delta)}^{-1}, \sqrt{V_{v(\Delta)}^\epsilon}\}), \end{aligned}$$

where $\epsilon(s_I s_J s_K) := \text{sgn}(\det(\dot{s}_I \dot{s}_J \dot{s}_K)(v))$ takes the values $+1, -1, 0$ if the tangents of the three segments s_I, s_J, s_K at v (in that sequence) form a matrix of positive, negative or vanishing determinant. Then the integration over Σ can be split as follows [2]:

$$\begin{aligned} \int_\Sigma &= \int_{\bar{U}_\alpha^\epsilon} + \sum_{v \in V(\alpha)} \int_{U_{\alpha, v}^\epsilon} \\ &= \int_{\bar{U}_\alpha^\epsilon} + \sum_{v \in V(\alpha)} \frac{1}{E(v)} \sum_{b(e_I) \cap b(e_J) \cap b(e_K) = v} \left[\int_{U_{\alpha, v, e_I, e_J, e_K}^\epsilon} + \int_{\bar{U}_{\alpha, v, e_I, e_J, e_K}^\epsilon} \right] \\ &\approx \int_{\bar{U}_\alpha^\epsilon} + \sum_{v \in V(\alpha)} \frac{1}{E(v)} \sum_{b(e_I) \cap b(e_J) \cap b(e_K) = v} \left[8 \cdot \int_{\Delta_{\alpha, v, e_I, e_J, e_K}^\epsilon} + \int_{\bar{U}_{\alpha, v, e_I, e_J, e_K}^\epsilon} \right]. \end{aligned}$$

Here we have first decomposed Σ into a region \bar{U}_α^ϵ not containing the vertices of α and the regions $U_{\alpha, v}^\epsilon$ around the vertices. Then choose a triple (e_I, e_J, e_K) of edges outgoing from v and decompose $U_{\alpha, v}^\epsilon$ into the region $U_{\alpha, v, e_I, e_J, e_K}^\epsilon$ covered by the tetrahedron $\Delta_{\alpha, v, e_I, e_J, e_K}^\epsilon$ spanned by e_I, e_J, e_K and its 7 mirror images and the rest $\bar{U}_{\alpha, v, e_I, e_J, e_K}^\epsilon$ not containing v . Note that the integral over $U_{\alpha, v, e_I, e_J, e_K}^\epsilon$ classically converges to 8 times the integral over the original single tetrahedron $\Delta_{\alpha, v, e_I, e_J, e_K}^\epsilon$ as we shrink the tetrahedron to zero. We average over all such triples (e_I, e_J, e_K) and divide by the number of possible choices of triples for a vertex v with $n(v)$ edges, $E(v) = \binom{n(v)}{3}$. Then by the above triangulation $T(\epsilon)$, the regulated 3 terms become

respectively

$$\begin{aligned} H_4^\epsilon &= -\lim_{\epsilon \rightarrow 0} \frac{2^{20}}{3^6 \gamma^6} \int_\Sigma d^3 y \pi(y) \\ &\times \sum_{v \in \alpha(v)} \frac{N(v(\Delta))}{E(v)} \sum_{v(\Delta)=v} \chi_\epsilon(v(\Delta'') - y) \chi_\epsilon(v(\Delta) - y) \\ &\times \text{Tr}(\tau_i h_{s_L(\Delta)} \{h_{s_L(\Delta)}^{-1}, \tilde{K}\}) \\ &\times \epsilon^{LMN} \epsilon(s_L s_M s_N) \text{Tr}(\tau_i h_{s_M(\Delta)} \{h_{s_M(\Delta)}^{-1}, (V_{U_{v(\Delta)}^\epsilon})^{3/4}\}) \\ &\times h_{s_N(\Delta)} \{h_{s_N(\Delta)}^{-1}, (V_{U_{v(\Delta)}^\epsilon})^{3/4}\}) \\ &\times \sum_{v'' \in \alpha(v)} \frac{1}{E(v'')} \sum_{v(\Delta)=v''} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \text{Tr}(h_{s_I(\Delta'')} \{h_{s_I(\Delta'')}^{-1}, \sqrt{V_{U_{v(\Delta'')}^\epsilon}}\} h_{s_J(\Delta'')} \{h_{s_J(\Delta'')}^{-1}, \sqrt{V_{U_{v(\Delta'')}^\epsilon}}\} \\ &\times h_{s_K(\Delta'')} \{h_{s_K(\Delta'')}^{-1}, \sqrt{V_{U_{v(\Delta'')}^\epsilon}}\}), \end{aligned}$$

$$\begin{aligned} H_5^\epsilon &= \lim_{\epsilon \rightarrow 0} \frac{2^{17}}{3^5 \gamma^6} \\ &\times \int_\Sigma d^3 x N(x) \phi(x) \pi(x) \int_\Sigma d^3 y \pi(y) \\ &\times \chi_\epsilon(v(\Delta''') - y) \chi_\epsilon(v(\Delta'') - x) \chi_\epsilon(x - y) \\ &\times \sum_{v'' \in \alpha(v)} \frac{1}{E(v'')} \sum_{v(\Delta)=v''} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \text{Tr}(h_{s_I(\Delta'')} \{h_{s_I(\Delta'')}^{-1}, \sqrt{V_{U_{v(\Delta'')}^\epsilon}}\} h_{s_J(\Delta'')} \{h_{s_J(\Delta'')}^{-1}, \sqrt{V_{U_{v(\Delta'')}^\epsilon}}\} \\ &\times h_{s_K(\Delta'')} \{h_{s_K(\Delta'')}^{-1}, \sqrt{V_{U_{v(\Delta'')}^\epsilon}}\}) \\ &\times \sum_{v''' \in \alpha(v)} \frac{1}{E(v''')} \sum_{v(\Delta)=v'''} \epsilon(s_L s_M s_N) \epsilon^{LMN} \\ &\times \text{Tr}(h_{s_L(\Delta''')} \{h_{s_L(\Delta''')}^{-1}, \sqrt{V_{U_{v(\Delta''')}^\epsilon}}\} h_{s_M(\Delta''')} \{h_{s_M(\Delta''')}^{-1}, \sqrt{V_{U_{v(\Delta''')}^\epsilon}}\} \\ &\times h_{s_N(\Delta''')} \{h_{s_N(\Delta''')}^{-1}, \sqrt{V_{U_{v(\Delta''')}^\epsilon}}\}), \end{aligned}$$

$$\begin{aligned} (79) \quad H_7^\epsilon &= -\lim_{\epsilon \rightarrow 0} \frac{2^7}{3 \gamma^2 i \lambda_0} \int_\Sigma d^3 x (D_a \chi_\epsilon(x - v')) N(x) E_i^a(x) \\ &\times \sum_{v' \in \alpha(v)} \frac{1}{E(v')} \sum_{v(\Delta')=v'} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times U_{\lambda_0}^{-1}(\phi(s_{s_I(\Delta')})) [U_{\lambda_0}(\phi(t_{s_I(\Delta')})) - U_{\lambda_0}(\phi(s_{s_I(\Delta')}))] \\ &\times \text{Tr}(\tau_i h_{s_J(\Delta')} \{h_{s_J(\Delta')}^{-1}, (V_{U_{\Delta'}^\epsilon})^{1/2}\} h_{s_K(\Delta')} \{h_{s_K(\Delta')}^{-1}, (V_{U_{\Delta'}^\epsilon})^{1/2}\}), \end{aligned} \quad (80)$$

where $v(\Delta)$ and $s_I(\Delta)$ denotes a vertex and a segment of a tetrahedron respectively, and $t_{s_I(\Delta)}$ ($s_{s_I(\Delta)}$) denotes target point (starting point) of a segment $s_I(\Delta)$. Note that the action of the operator $\pi(R)$ on a scalar-network basis vector $T_X(\phi)$ over a graph X can be factorized as

$$\hat{\pi}(R) \cdot T_X = \sum_{x_i \in X \cap R} \hat{\pi}_{x_i} \cdot T_X. \quad (81)$$

Now every ingredient of H_i^ε has clearly quantum analogy, we can define the corresponding operators acting on a basis vector $T_{\alpha,X}$ over some graph $\alpha \cup X$ as

$$\begin{aligned} \hat{H}_4^\varepsilon \cdot T_{\alpha,X} &= -\lim_{\varepsilon \rightarrow 0} \frac{2^{20}}{3^6 \gamma^6 (i\hbar)^6} \\ &\times \sum_{v' \in X} \hat{\pi}(v') \chi_\varepsilon(v'' - v') \chi_\varepsilon(v' - v) \\ &\times \sum_{v \in \alpha(v)} \frac{N(v)}{E(v)} \sum_{v(\Delta)=v} \text{Tr}(\tau_i \hat{h}_{s_L(\Delta_v)} [\hat{h}_{s_L(\Delta_v)}^{-1}, \hat{K}]) \\ &\times \epsilon(s_L s_M s_N) \epsilon^{LMN} \text{Tr}(\tau_i \hat{h}_{s_M(\Delta_v)} [\hat{h}_{s_M(\Delta_v)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{3/4}]) \\ &\times \hat{h}_{s_N(\Delta_v)} [\hat{h}_{s_N(\Delta_v)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{3/4}]) \\ &\times \sum_{v'' \in \alpha(v)} \frac{1}{E(v'')} \sum_{v(\Delta)=v''} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \text{Tr}(\hat{h}_{s_I(\Delta_{v''})} [\hat{h}_{s_I(\Delta_{v''})}^{-1}, (\hat{V}_{U_{v''}^\varepsilon})^{1/2}]) \\ &\times \hat{h}_{s_J(\Delta_{v''})} [\hat{h}_{s_J(\Delta_{v''})}^{-1}, (\hat{V}_{U_{v''}^\varepsilon})^{1/2}]) \\ &\times \hat{h}_{s_K(\Delta_{v''})} [\hat{h}_{s_K(\Delta_{v''})}^{-1}, (\hat{V}_{U_{v''}^\varepsilon})^{1/2}]) \cdot T_{\alpha,X}, \end{aligned} \quad (82)$$

$$\begin{aligned} \hat{H}_5^\varepsilon \cdot T_{\alpha,X} &= \lim_{\varepsilon \rightarrow 0} \frac{2^{18}}{3^5 \gamma^6 (i\hbar)^6} \sum_{v \in X} \sum_{v' \in X} \\ &\times \hat{\phi}(v) N(v) \hat{\pi}(v') \chi_\varepsilon(v'' - v') \chi_\varepsilon(v'' - v) \chi_\varepsilon(v' - v) \\ &\times \sum_{v'' \in \alpha(v)} \frac{1}{E(v'')} \sum_{v(\Delta)=v''} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \text{Tr}(\hat{h}_{s_I(\Delta_{v''})} [\hat{h}_{s_I(\Delta_{v''})}^{-1}, (\hat{V}_{U_{v''}^\varepsilon})^{1/2}]) \\ &\times \hat{h}_{s_J(\Delta_{v''})} [\hat{h}_{s_J(\Delta_{v''})}^{-1}, (\hat{V}_{U_{v''}^\varepsilon})^{1/2}]) \\ &\times \hat{h}_{s_K(\Delta_{v''})} [\hat{h}_{s_K(\Delta_{v''})}^{-1}, (\hat{V}_{U_{v''}^\varepsilon})^{1/2}]) \\ &\times \sum_{v''' \in \alpha(v)} \frac{1}{E(v''')} \sum_{v(\Delta)=v'''} \epsilon(s_L s_M s_N) \epsilon^{LMN} \\ &\times \text{Tr}(\hat{h}_{s_L(\Delta_{v'''})} [\hat{h}_{s_L(\Delta_{v'''})}^{-1}, (\hat{V}_{U_{v'''}})^{1/2}]) \\ &\times \hat{h}_{s_M(\Delta_{v'''})} [\hat{h}_{s_M(\Delta_{v'''})}^{-1}, (\hat{V}_{U_{v'''}})^{1/2}]) \\ &\times \hat{h}_{s_N(\Delta_{v'''})} [\hat{h}_{s_N(\Delta_{v'''})}^{-1}, (\hat{V}_{U_{v'''}})^{1/2}]) \cdot T_{\alpha,X}, \end{aligned} \quad (83)$$

$$\begin{aligned} \hat{H}_7^\varepsilon \cdot T_{\alpha,X} &= -\lim_{\varepsilon \rightarrow 0} \frac{2^7}{3 \gamma^2 i \lambda_0} \sum_{e \in E(\alpha)} X_e^i(t_{k-1}) \lim_{n \rightarrow \infty} \sum_{k=1}^n \\ &\times [\chi_\varepsilon(e(t_k) - v') - \chi_\varepsilon(e(t_{k-1}) - v')] N(e(t_{k-1})) \\ &\times \sum_{v' \in \alpha(v)} \frac{1}{E(v')} \sum_{v(\Delta)=v'} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \hat{U}_{\lambda_0}^{-1}(\phi(s_{s_I(\Delta_{v'})})) [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta_{v'})})) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta_{v'})}))] \\ &\times \text{Tr}(\tau_i \hat{h}_{s_J(\Delta_{v'})} [\hat{h}_{s_J(\Delta_{v'})}^{-1}, (\hat{V}_{U_{v'}^\varepsilon})^{1/2}]) \\ &\times \hat{h}_{s_K(\Delta_{v'})} [\hat{h}_{s_K(\Delta_{v'})}^{-1}, (\hat{V}_{U_{v'}^\varepsilon})^{1/2}]) \cdot T_{\alpha,X}, \end{aligned} \quad (84)$$

where $0 = t_0 < t_1 < \dots < t_n = 1$ is an arbitrary partition of the interval $[0, 1]$, $X_e^i(t) := [h_e(0, t) \tau_i h_e(t, 1)]_{AB} \partial / \partial [h_e(0, 1)]_{AB}$

(we denote $X_e^i := X_e^i(0)$ in the following), and $h_{s_I(\Delta_v)}$ denotes the holonomy along the segment s_I starting from the vertex v of tetrahedron Δ . On the other hand, for \hat{H}_7^ε , we perform the limit $n \rightarrow \infty$, and $\varepsilon \rightarrow 0$ in reversed order. Keeping n fixed, for small enough ε , only the term with $k = 1$ in the sum survives provided that $s_I(0) = v'$. So for small enough ε , the above operator reduces to

$$\begin{aligned} \hat{H}_7^\varepsilon \cdot T_{\alpha,X} &= \lim_{\varepsilon \rightarrow 0} \frac{2^7}{3 \gamma^2 i \lambda_0 (i\hbar)^2} \\ &\times \sum_{e \in E(\alpha)} X_e^i(0) \chi_\varepsilon(e(0) - v') N(e(0)) \\ &\times \sum_{v' \in \alpha(v)} \frac{1}{E(v')} \sum_{v(\Delta)=v'} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \hat{U}_{\lambda_0}^{-1}(\phi(s_{s_I(\Delta_{v'})})) [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta_{v'})})) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta_{v'})}))] \\ &\times \text{Tr}(\tau_i \hat{h}_{s_J(\Delta_{v'})} [\hat{h}_{s_J(\Delta_{v'})}^{-1}, (\hat{V}_{U_{v'}^\varepsilon})^{1/2}]) \\ &\times \hat{h}_{s_K(\Delta_{v'})} [\hat{h}_{s_K(\Delta_{v'})}^{-1}, (\hat{V}_{U_{v'}^\varepsilon})^{1/2}]) \cdot T_{\alpha,X}. \end{aligned} \quad (85)$$

Since the actions of \hat{H}_4^ε and \hat{H}_5^ε are independent of ε , we can take the limits and obtain

$$\begin{aligned} \hat{H}_4 \cdot T_{\alpha,X} &= - \sum_{v \in V(\alpha) \cap X} \frac{2^{20} N(v)}{3^6 \gamma^6 (i\hbar)^6 E^2(v)} \hat{\pi}(v) \\ &\times \sum_{v(\Delta)=v(\Delta')=v} \text{Tr}(\tau_i \hat{h}_{s_L(\Delta)} [\hat{h}_{s_L(\Delta)}^{-1}, \hat{K}]) \\ &\times \epsilon(s_L s_M s_N) \epsilon^{LMN} \\ &\times \text{Tr}(\tau_i \hat{h}_{s_M(\Delta)} [\hat{h}_{s_M(\Delta)}^{-1}, (\hat{V}_v)^{3/4}] \hat{h}_{s_N(\Delta)} [\hat{h}_{s_N(\Delta)}^{-1}, (\hat{V}_v)^{3/4}]) \\ &\times \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \text{Tr}(\hat{h}_{s_I(\Delta')} [\hat{h}_{s_I(\Delta')}^{-1}, (\hat{V}_v)^{1/2}] \hat{h}_{s_J(\Delta')} [\hat{h}_{s_J(\Delta')}^{-1}, (\hat{V}_v)^{1/2}]) \\ &\times \hat{h}_{s_K(\Delta')} [\hat{h}_{s_K(\Delta')}^{-1}, (\hat{V}_v)^{1/2}]) \cdot T_{\alpha,X}, \end{aligned} \quad (86)$$

$$\begin{aligned} \hat{H}_5 \cdot T_{\alpha,X} &= \sum_{v \in V(\alpha) \cap X} \frac{2^{18} N(v)}{3^5 \gamma^6 (i\hbar)^6 E^2(v)} \hat{\pi}(v) \hat{\phi}(v) \hat{\pi}(v) \\ &\times \sum_{v(\Delta)=v(\Delta')=v} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \text{Tr}(\hat{h}_{s_I(\Delta)} [\hat{h}_{s_I(\Delta)}^{-1}, (\hat{V}_v)^{1/2}] \hat{h}_{s_J(\Delta)} [\hat{h}_{s_J(\Delta)}^{-1}, (\hat{V}_v)^{1/2}]) \\ &\times \hat{h}_{s_K(\Delta)} [\hat{h}_{s_K(\Delta)}^{-1}, (\hat{V}_v)^{1/2}]) \\ &\times \epsilon(s_L s_M s_N) \epsilon^{LMN} \\ &\times \text{Tr}(\hat{h}_{s_L(\Delta')} [\hat{h}_{s_L(\Delta')}^{-1}, (\hat{V}_v)^{1/2}] \hat{h}_{s_M(\Delta')} [\hat{h}_{s_M(\Delta')}^{-1}, (\hat{V}_v)^{1/2}]) \\ &\times \hat{h}_{s_N(\Delta')} [\hat{h}_{s_N(\Delta')}^{-1}, (\hat{V}_v)^{1/2}]) \cdot T_{\alpha,X}. \end{aligned} \quad (87)$$

However, it is easy to see that the action of \hat{H}_7^ε on $T_{\alpha,X}$ is graph changing. It adds a finite number of vertices at $t(s_I(v)) = \varepsilon$ for edges $e_I(t)$ starting from each high-valent vertex of α . As a result, the family of operators $\hat{H}_7^\varepsilon(N)$ fails to be weakly convergent when $\varepsilon \rightarrow 0$. However, due to the diffeomorphism covariant properties of the triangulation, the limit operator can be well defined via the so-called uniform Rovelli-Smolín

topology induced by diffeomorphism-invariant states Φ_{Diff} as:

$$\Phi_{Diff}(\hat{H}_7 \cdot T_{\alpha,X}) = \lim_{\varepsilon \rightarrow 0} (\Phi_{Diff}|\hat{H}_7^\varepsilon|T_{\alpha,X}). \quad (88)$$

It is obviously that the limit is independent of ε . Hence both the regulators ε and ε can be removed. We then have

$$\begin{aligned} \hat{H}_7 \cdot T_{\alpha,X} &= \sum_{v \in V(\alpha)} \frac{2^7 N(v)}{3\gamma^2 i\lambda_0 (i\hbar)^2 E(v)} \\ &\times \sum_{e(0)=v} X_e^i \sum_{v(\Delta)=v} \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \hat{U}_{\lambda_0}^{-1}(\phi(s_{s_I(\Delta)})) [\hat{U}_{\lambda_0}(\phi(t_{s_I(\Delta)})) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta)}))] \\ &\times \text{Tr}(\tau_i \hat{h}_{s_J(\Delta)}) [\hat{h}_{s_J(\Delta)}^{-1}, (\hat{V}_v)^{1/2}] \\ &\times \hat{h}_{s_K(\Delta)} [\hat{h}_{s_K(\Delta)}^{-1}, (\hat{V}_v)^{1/2}] \cdot T_{\alpha,X}. \end{aligned} \quad (89)$$

Collecting all terms, the whole Hamiltonian constraint can be quantized as a well-defined operator $\hat{H}(N)$ in \mathcal{H}_{kin} . The action of $\hat{H}(N)$ on $T_{\alpha,X}$ can be factorized as

$$\hat{H}(N) \cdot T_{\alpha,X} = \sum_{v \in V(\alpha)} \hat{H}(N)_v \cdot T_{\alpha,X}. \quad (90)$$

This operator is internal gauge invariant and hence also well defined in \mathcal{H}_G . However, although $\hat{H}(N)$ can dually act on the diffeomorphism invariant states, there is no guarantee for the resulted states to be still diffeomorphism invariant.

V. MASTER CONSTRAINT OPERATOR

Although the Hamiltonian constraint operator constructed in last section is well defined in \mathcal{H}_G , it is difficult to define it directly on \mathcal{H}_{Diff} . Moreover, the constraint algebra (41)-(46) do not form a Lie algebra. This might lead to quantum anomaly after quantization. In order to avoid possible quantum anomaly and find the physical Hilbert space, master constraint programme was first introduced by Thiemann in [25]. We now apply this programme to quantum $f(\mathcal{R})$ gravity.

By definition the master constraint of $f(\mathcal{R})$ theories classically reads

$$\mathcal{M} := \frac{1}{2} \int_{\Sigma} d^3x \frac{|H(x)|^2}{\sqrt{h}}, \quad (91)$$

where the Hamiltonian constraint $H(x)$ was given by Eq.(39). It is obvious that

$$\mathcal{M} = 0 \Leftrightarrow H(N) = 0 \quad \forall N(x). \quad (92)$$

However, now the constraints form a Lie algebra since

$$\begin{aligned} \{\mathcal{V}(\vec{N}), \mathcal{V}(\vec{N}')\} &= \mathcal{V}([\vec{N}, \vec{N}']), \\ \{\mathcal{V}(\vec{N}), \mathcal{M}\} &= 0, \\ \{\mathcal{M}, \mathcal{M}\} &= 0, \end{aligned} \quad (93)$$

where diffeomorphism constraints nicely form an ideal. The master constraint can be regulated via a point-splitting strategy [26] as:

$$\mathcal{M}^\varepsilon = \frac{1}{2} \int_{\Sigma} d^3y \int_{\Sigma} d^3x \chi_\varepsilon(x-y) \frac{H(x)}{\sqrt{V_{U_x^\varepsilon}}} \frac{H(y)}{\sqrt{V_{U_y^\varepsilon}}}. \quad (94)$$

Introducing a partition \mathcal{P} of the 3-manifold Σ into cells C , we have an operator $\hat{H}_{C,\beta}^\varepsilon$ acting on spin-scalar-network basis $T_{s,c}$ in \mathcal{H}_G via a state-dependent triangulation,

$$\hat{H}_{C,\alpha}^\varepsilon \cdot T_{s,c} = \sum_{v \in V(\alpha)} \chi_C(v) \hat{H}(N)_v^\varepsilon \cdot T_{s,c} \quad (95)$$

where α denotes the underlying graph of the spin-network state T_s , and

$$\hat{H}(N)_v^\varepsilon = \sum_{v(\Delta)=v} \hat{H}_{GR,v}^{\varepsilon,\Delta} + \sum_{i=3}^7 \hat{H}_{i,v}^\varepsilon, \quad (96)$$

with

$$\begin{aligned} \hat{H}_{GR,v}^{\varepsilon,\Delta} &= \frac{32\hat{\phi}(v)}{3i\hbar\gamma E(v)} \epsilon(s_I s_J s_K) \epsilon^{IJK} \text{Tr}(\hat{h}_{s_I(\Delta)}^{-1} \hat{h}_{s_J(\Delta)} [\hat{h}_{s_K(\Delta)}^{-1}, \sqrt{\hat{V}_{U_v^\varepsilon}}]) \\ &- \frac{64}{(i\hbar)^3 \gamma^3 E(v)} (\hat{\phi}^{-1}(v) + \gamma^2 \hat{\phi}(v)) \epsilon(s_I s_J s_K) \epsilon^{IJK} \\ &\times \text{Tr}(\hat{h}_{s_I(\Delta)} [\hat{h}_{s_I(\Delta)}^{-1}, \hat{K}] \hat{h}_{s_J(\Delta)} [\hat{h}_{s_J(\Delta)}^{-1}, \hat{K}] \hat{h}_{s_K(\Delta)} [\hat{h}_{s_K(\Delta)}^{-1}, \sqrt{\hat{V}_{U_v^\varepsilon}}]), \end{aligned} \quad (97)$$

and

$$\begin{aligned} \hat{H}_{3,v}^\varepsilon &= \frac{16N(v)}{3\gamma^3 (i\hbar)^2} \hat{\phi}^{-1}(v) \\ &\times [H^{\hat{E}ucl}(1), (\hat{V}_{U_v^\varepsilon})^{1/4}] [H^{\hat{E}ucl}(1), (\hat{V}_{U_v^\varepsilon})^{1/4}], \end{aligned} \quad (98)$$

$$\begin{aligned} \hat{H}_{4,v}^\varepsilon &= - \sum_{v(\Delta)=v(\Delta')=v(X)=v} \frac{2^{18}N(v)}{3^4 \gamma^6 (i\hbar)^6 E^2(v)} \hat{\pi}(v) \\ &\times \text{Tr}(\tau_i \hat{h}_{s_L(\Delta)} [\hat{h}_{s_L(\Delta)}^{-1}, \hat{K}]) \\ &\times \epsilon(s_L s_M s_N) \epsilon^{LMN} \text{Tr}(\tau_i \hat{h}_{s_M(\Delta)} [\hat{h}_{s_M(\Delta)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}]) \\ &\times \hat{h}_{s_N(\Delta)} [\hat{h}_{s_N(\Delta)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}] \\ &\times \epsilon(s_I s_J s_K) \epsilon^{IJK} \text{Tr}(\hat{h}_{s_I(\Delta')} [\hat{h}_{s_I(\Delta')}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}]) \\ &\times \hat{h}_{s_J(\Delta')} [\hat{h}_{s_J(\Delta')}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}] \\ &\times \hat{h}_{s_K(\Delta')} [\hat{h}_{s_K(\Delta')}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}], \end{aligned} \quad (99)$$

$$\begin{aligned}
\hat{H}_{5,v}^\varepsilon = & \sum_{v(\Delta)=v(\Delta')=v(X)=v} \frac{2^{20}N(v)}{3^5\gamma^6(i\hbar)^6E^2(v)} \hat{\pi}(v)\hat{\phi}(v)\hat{\pi}(v) \\
& \times \epsilon(s_I s_J s_K) \epsilon^{IJK} \text{Tr}(\hat{h}_{s_I(\Delta)}[\hat{h}_{s_I(\Delta)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/4}] \\
& \times \hat{h}_{s_J(\Delta)}[\hat{h}_{s_J(\Delta)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}] \\
& \times \hat{h}_{s_K(\Delta)}[\hat{h}_{s_K(\Delta)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}]) \\
& \times \epsilon(s_L s_M s_N) \epsilon^{LMN} \text{Tr}(\hat{h}_{s_L(\Delta')}[\hat{h}_{s_L(\Delta')}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/4}] \\
& \times \hat{h}_{s_M(\Delta')}[\hat{h}_{s_M(\Delta')}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}] \\
& \times \hat{h}_{s_N(\Delta')}[\hat{h}_{s_N(\Delta')}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/2}]),
\end{aligned} \tag{100}$$

$$\hat{H}_{6,v}^\varepsilon = \frac{1}{2}N(v)\hat{\xi}(\phi(v))\sqrt{\hat{V}_{U_v^\varepsilon}}, \tag{101}$$

$$\begin{aligned}
\hat{H}_{7,v}^\varepsilon = & \frac{2^9}{3\gamma^2 i\lambda_0 (i\hbar)^2 E(v)} \\
& \times \sum_{e(0)=v} X_e^i \sum_{v(\Delta)=v} \\
& \times \epsilon(s_I s_J s_K) \epsilon^{IJK} \hat{U}_{\lambda_0}^{-1}(\phi(s_{s_I(\Delta)})) \\
& \times [\hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta)})) - \hat{U}_{\lambda_0}(\phi(s_{s_J(\Delta)}))] \\
& \times \text{Tr}(\tau_i \hat{h}_{s_J(\Delta)}[\hat{h}_{s_J(\Delta)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/4}] \\
& \times \hat{h}_{s_K(\Delta)}[\hat{h}_{s_K(\Delta)}^{-1}, (\hat{V}_{U_v^\varepsilon})^{1/4}]).
\end{aligned} \tag{102}$$

Note that the family of operators $\hat{H}_{C,\alpha}^\varepsilon$ are cylindrically consistent up to diffeomorphism. So the inductive limit operator \hat{H}_C is densely defined in \mathcal{H}_G by the uniform Rovelli- Smolin topology. Moreover, the adjoint operators of $\hat{H}_{C,\alpha}^\varepsilon$, which are also cylindrically consistent up to diffeomorphism, read

$$(\hat{H}_{C,\alpha}^\varepsilon)^\dagger \cdot T_{s,c} = \sum_{v \in V(\alpha)} \chi_C(v) (\hat{H}(N_v^\varepsilon)^\dagger \cdot T_{s,c}) \tag{103}$$

The inductive limit operator, $(\hat{H}_C)^\dagger$, of $(\hat{H}_{C,\alpha}^\varepsilon)^\dagger$ is adjoint to \hat{H}_C . Then we could define master constraint operator $\hat{\mathcal{M}}$ on diffeomorphism invariant states as

$$(\hat{\mathcal{M}}\Phi_{Diff}) \cdot T_{s,c} = \lim_{\mathcal{P} \rightarrow \Sigma, \varepsilon, \varepsilon' \rightarrow 0} \Phi_{Diff}[\frac{1}{2} \sum_{c \in \mathcal{P}} \hat{H}_C^\varepsilon (\hat{H}_C^{\varepsilon'})^\dagger \cdot T_{s,c}] \tag{104}$$

Note that our construction of $\hat{\mathcal{M}}$ is qualitatively similar to that in [27], although the quantitative actions are different. Similar to those in [27] we can prove the following properties of $\hat{\mathcal{M}}$.

(i) $\hat{\mathcal{M}}$ is diffeomorphism invariant, i.e.,

$$(\hat{U}'_\varphi \hat{\mathcal{M}}\Phi_{Diff}) \cdot T_{s,c} = (\hat{\mathcal{M}}\Phi_{Diff}) \cdot T_{s,c},$$

where \hat{U}'_φ is induced by the unitary operator in \mathcal{H}_G corresponding to a finite diffeomorphism transformation φ .

(ii) For any given diffeomorphism invariant spin-scalar-network state $T_{[s,c]}$, the norm $\|\hat{\mathcal{M}}T_{[s,c]}\|_{Diff}$ is finite. So $\hat{\mathcal{M}}$ is densely defined in \mathcal{H}_{Diff} .

(iii) $\hat{\mathcal{M}}$ is a positive and symmetric operator in \mathcal{H}_{Diff} and hence admits a unique self-adjoint Friedrichs extension.

In conclusion, there exists a positive and self-adjoint operator $\hat{\mathcal{M}}$ on \mathcal{H}_{Diff} corresponding to the master constraint (91). It is then possible to obtain the physical Hilbert space of $f(\mathcal{R})$ gravity by the direct integral decomposition of \mathcal{H}_{Diff} with respect to $\hat{\mathcal{M}}$.

VI. CONCLUDING REMARKS

How to unify quantum mechanics with gravity theory is one of the core problems in modern physics. In recent twenty-five years, LQG has made considerable progress in quantizing GR non-perturbatively and hence become a fascinating candidate theory for quantum gravity. This background-independent quantization relies on the key observation that classical GR can be cast into the connection-dynamical formalism with the structure group of $SU(2)$. Due to this particular formalism, LQG was generally considered as a quantization scheme that applies only to GR. This was taken by many researchers to be a limitation of the quantization scheme. The fact of being of general applicability would therefore be significant for the general debate about quantum gravity. Especially, $f(\mathcal{R})$ gravity theories have become topical in issues related to dark energy in cosmology and non-trivial astronomic tests beyond GR. Hence, whether such modified gravity theories could be quantized non-perturbatively is itself an interesting question.

The main results of Ref.[10] and the current paper can be summarized as follows. (i) The connection dynamics of $f(\mathcal{R})$ gravity has been obtained by canonical transformations from its geometric dynamics. (ii) Based on the $su(2)$ -connection dynamical formalism, the rigorous kinematical framework of LQG has been successfully extended to metric $f(\mathcal{R})$ gravity theories by coupling with a polymer-like scalar field. The important physical result that both the area and the volume are discrete at quantum kinematical level remains valid for $f(\mathcal{R})$ gravity. (iii) While the Hamiltonian constraint is promoted to well-defined operator in the kinematical Hilbert space, the master constraint can be promoted to well-defined operator in the diffeomorphism invariant Hilbert space of loop quantum $f(\mathcal{R})$ gravity. Thus, the non-perturbative loop quantization procedure is not only valid for GR but also valid for a rather general class of 4-dimensional metric theories of gravity. Therefore, the achievements which have been obtained are in two fold. First, classical metric $f(\mathcal{R})$ theories have been successfully quantized non-perturbatively. This guarantees the existence of $f(\mathcal{R})$ theories of gravity at fundamental quantum level. Secondly, the valid range of LQG has been considerably enlarged to include a rather general class of metric theories.

It should be noticed that classically the scalar field ϕ characterize different $f(\mathcal{R})$ theories of gravity by $\phi = f'(\mathcal{R})$. Thus for a given $f(\mathcal{R})$ theory, ϕ becomes a particular function of scalar curvature \mathcal{R} while the potential $\xi(\phi)$ is fixed. Hence our quan-

tum $f(\mathcal{R})$ gravity may be understood as a class of quantum theories representing different choices of the function $f(\mathcal{R})$. Of course, there are still many aspects of the connection formalism and loop quantization of $f(\mathcal{R})$ theories which deserve discovering. For examples, it is still desirable to find an action for the connection dynamics of $f(\mathcal{R})$ gravity. The semiclassical analysis of loop quantum $f(\mathcal{R})$ theories is yet to be done. To further explore the physical contents of the loop quantum $f(\mathcal{R})$ gravity, we would like to study its applications to cosmology and black holes in future works. Moreover, It is also desirable to quantize $f(\mathcal{R})$ theories by covariant spin foam approach.

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Appendix

We use (\tilde{K}_a^i, E_j^b) and (ϕ, π) as canonical variables to derive the constraints algebra. By the first canonical transformation, The Hamiltonian constraint (12) in section II can be written as

$$\begin{aligned} H &= \frac{\sqrt{h}}{2\phi}[(\tilde{K}_{ab}\tilde{K}^{ab} - \tilde{K}^2) - \phi^2 R] - \frac{2}{3\sqrt{h}}(\pi p - \frac{p^2}{\phi}) \\ &+ \frac{1}{3}\frac{\pi^2\phi}{\sqrt{h}} + \frac{1}{2}\sqrt{h}\xi(\phi) + \sqrt{h}D_a D^a \phi, \\ &= \frac{1}{2\sqrt{h}\phi}(\tilde{K}_a^i E_i^b \tilde{K}_b^j E_j^a - \frac{1}{3}\tilde{K}_a^i E_i^a \tilde{K}_b^j E_j^b) - \frac{1}{2}\phi\sqrt{h}R + \frac{1}{2}\sqrt{h}\xi(\phi) \\ &+ \frac{1}{2\sqrt{h}}(\frac{4}{3}\tilde{K}_a^i E_i^a \pi + \frac{2}{3}\pi^2\phi) + \sqrt{h}D_a D^a \phi. \end{aligned} \quad (105)$$

To calculate the Poisson bracket between two smeared Hamiltonian constraints, we notice that the non-vanishing contributions come only from the terms which contain the derivative of canonical variables. Those terms are $\int_\Sigma d^3x N \sqrt{h} D_a D^a \phi$, which contains both the derivative of E_j^b and the derivative of ϕ , and $\int_\Sigma -\frac{1}{2}\phi N \sqrt{h} R$, which only contain the derivative of E_j^b . Hence we first use $\{\phi(x), \pi(y)\} = \delta^3(x, y)$ to calculate

$$\begin{aligned} &\{ \int_\Sigma N \sqrt{h} D_a D^a \phi, \int_\Sigma \frac{M}{2\sqrt{h}}(\frac{4}{3}\tilde{K}_a^i E_i^a \pi + \frac{2}{3}\pi^2\phi) \}_{(\phi, \pi)} - M \leftrightarrow N \\ &= \int_\Sigma (M D_a D^a N - N D_a D^a M)(\frac{2}{3}\pi\phi + \frac{2}{3}\tilde{K}_b^j E_j^b) \\ &= \int_\Sigma (N D^a M - M D^a N) D_a (\frac{2}{3}\pi\phi + \frac{2}{3}\tilde{K}_b^j E_j^b). \end{aligned} \quad (106)$$

Note also that

$$N \sqrt{h} D_a D^a \phi = N \sqrt{h} h^{ab} (\partial_a \partial_b \phi - \Gamma_{ab}^c \partial_c \phi). \quad (107)$$

Since only Γ_{ab}^c contains the derivative of E_i^a in above equation, we consider

$$\begin{aligned} &N \sqrt{h} h^{ab} \Gamma_{ab}^c \partial_c \phi \\ &= \frac{N}{2} \sqrt{h} h^{ab} (\partial_c \phi) (h^{cd} (-\partial_a h_{bd} - \partial_b h_{ad} + \partial_a h_{ab})) \\ &= \frac{N}{2} \sqrt{h} (\partial_c \phi) (2\partial_a h^{ac} - h_{ab} \partial^c h^{ab}) \\ &= \frac{N}{2} \sqrt{h} (\partial_c \phi) (2\partial_a (\frac{E_i^a E_i^c}{h}) - h_{ab} \partial^c (\frac{E_i^a E_i^b}{h})). \end{aligned} \quad (108)$$

Therefore, we use $\{\tilde{K}_a^j(x), E_k^b(y)\} = \delta_a^b \delta_k^j \delta(x, y)$ to calculate

$$\begin{aligned} &\{ \int_\Sigma N \sqrt{h} (\partial_c \phi) \partial_a (\frac{E_i^a E_i^c}{h}), \int_\Sigma \frac{M}{2\sqrt{h}} (\frac{1}{\phi} (\tilde{K}_d^l E_l^b \tilde{K}_b^j E_j^d \\ &- \frac{1}{3} \tilde{K}_d^l E_l^d \tilde{K}_b^j E_j^b) + \frac{4}{3} \tilde{K}_d^l E_l^d \pi) \}_{(\tilde{K}, E)} - M \leftrightarrow N \\ &= \int_\Sigma \frac{1}{2} M (\partial_a N) (D_c \phi) \frac{2E_i^c}{h} (\frac{2}{\phi} (E_i^b \tilde{K}_b^j E_j^a \\ &- \frac{1}{3} E_i^a \tilde{K}_b^j E_j^b) + \frac{4}{3} E_i^a \pi)) \\ &+ \frac{1}{2} M (\partial_a N) (D_c \phi) \frac{E_i^a E_i^c}{h} (-E_j^j) (\frac{2}{\phi} (E_j^b \tilde{K}_b^m E_m^d \\ &- \frac{1}{3} E_j^d \tilde{K}_b^m E_m^b) + \frac{4}{3} E_j^d \pi)) - M \leftrightarrow N \end{aligned} \quad (109)$$

and

$$\begin{aligned} &\{ \int_\Sigma -\frac{N}{2} \sqrt{h} (\partial_c \phi) h_{ae} \partial^c (\frac{E_i^a E_i^e}{h}), \int_\Sigma \frac{M}{2\sqrt{h}} (\frac{1}{\phi} (\tilde{K}_d^l E_l^b \tilde{K}_b^j E_j^d \\ &- \frac{1}{3} \tilde{K}_d^l E_l^d \tilde{K}_b^j E_j^b) + \frac{4}{3} \tilde{K}_d^l E_l^d \pi) \}_{(\tilde{K}, E)} - M \leftrightarrow N \\ &= \int_\Sigma -\frac{1}{4} M (\partial^c N) (D_c \phi) h_{ae} \frac{2E_i^e}{h} (\frac{2}{\phi} (E_i^b \tilde{K}_b^j E_j^a \\ &- \frac{1}{3} E_i^a \tilde{K}_b^j E_j^b) + \frac{4}{3} E_i^a \pi)) \\ &- \frac{1}{4} M (\partial_a N) (D_c \phi) \frac{E_i^a E_i^c}{h} (-3E_j^j) (\frac{2}{\phi} (E_j^b \tilde{K}_b^m E_m^d \\ &- \frac{1}{3} E_j^d \tilde{K}_b^m E_m^b) + \frac{4}{3} E_j^d \pi)) - M \leftrightarrow N. \end{aligned} \quad (110)$$

The combination of above two Poisson brackets equals to

$$\begin{aligned} &\int_\Sigma (N D^a M - M D^a N) (-\frac{1}{3} \pi D_a \phi \\ &- \frac{2}{\phi} (\tilde{K}_b^j E_j^b h_{ac} D^b \phi - \frac{1}{3} \tilde{K}_b^j E_j^b D_a \phi)). \end{aligned} \quad (111)$$

The variation of the terms containing a derivative in $\int_{\Sigma} -\frac{1}{2}\phi N \sqrt{h}R$ reads

$$\begin{aligned} & \int_{\Sigma} \frac{1}{2} \sqrt{h} (-D^a D^b (\phi N) + h^{ab} D_c D^c (\phi N)) \delta h_{ab} \\ &= \int_{\Sigma} \frac{1}{2} \sqrt{h} (D_a D_b (\phi N) - h_{ab} D_c D^c (\phi N)) \delta h^{ab} \\ &= \int_{\Sigma} \frac{1}{2} \sqrt{h} (D_a D_b (\phi N) - h_{ab} D_c D^c (\phi N)) \delta \left(\frac{E_i^a E_i^b}{h} \right). \end{aligned} \quad (112)$$

Thus we have

$$\begin{aligned} & \left\{ \int_{\Sigma} -\frac{1}{2} \phi N \sqrt{h} R, \int_{\Sigma} \frac{M}{2\sqrt{h}} \left(\frac{1}{\phi} (\tilde{K}_d^l E_l^e \tilde{K}_e^j E_j^d \right. \right. \\ & \left. \left. - \frac{1}{3} \tilde{K}_d^j E_j^d \tilde{K}_e^m E_m^e) + \frac{4}{3} \tilde{K}_d^l E_l^d \pi \right) \right\} - M \leftrightarrow N \\ &= \int_{\Sigma} -\frac{1}{4} (M D_a D_b (\phi N) - h_{ab} M D_c D^c (\phi N)) \frac{2E_i^b}{h} \\ & \quad \left(\frac{2}{\phi} (E_i^e \tilde{K}_e^j E_j^a - \frac{1}{3} \tilde{K}_d^j E_j^d E_i^a) + \frac{4}{3} E_i^a \pi \right) \\ & \quad - \frac{1}{4} (-2 M D_c D^c (\phi N)) (-E_i^a) \left(\frac{2}{\phi} (E_i^e \tilde{K}_e^j E_j^a \right. \\ & \quad \left. - \frac{1}{3} \tilde{K}_d^j E_j^d E_i^a) + \frac{4}{3} E_i^a \pi \right) - M \leftrightarrow N \\ &= \int_{\Sigma} - (M D_a D_b (\phi N) - h_{ab} M D_c D^c (\phi N)) h^{be} \frac{1}{\phi} \tilde{K}_e^j E_j^a \\ & \quad - M (D_c D^c \phi N) \left(\frac{2}{3\phi} \tilde{K}_d^j E_j^d + \frac{2}{3} \pi \right) - M \leftrightarrow N \\ &= \int_{\Sigma} - M (D_a D^b \phi N) \frac{1}{\phi} \tilde{K}_b^j E_j^a + M (D_c D^c \phi N) \\ & \quad \left(\frac{1}{3\phi} \tilde{K}_d^j E_j^d - \frac{2}{3} \pi \right) - M \leftrightarrow N \\ &= \int_{\Sigma} (N D_a D^b (\phi M) - M D_a D^b (\phi N)) \frac{1}{\phi} \tilde{K}_b^j E_j^a \\ & \quad + (N D_c D^c (\phi M) - M D_c D^c (\phi N)) \left(\frac{2}{3} \pi - \frac{1}{3\phi} \tilde{K}_d^j E_j^d \right) \\ &= \int_{\Sigma} (N D_c D^c M - M D_c D^c N) \left(\frac{2}{3} \pi \phi - \frac{1}{3} \tilde{K}_d^j E_j^a \right) \\ & \quad + (N D_c M - M D_c N) (D^c \phi) \left(\frac{4}{3} \pi - \frac{2}{3\phi} \tilde{K}_d^j E_j^a \right) \\ & \quad + (N D_a D^b M - M D_a D^b N) \tilde{K}_b^j E_j^a \\ & \quad + (N D_a M - M D_a N) \frac{2D^b \phi}{\phi} \tilde{K}_b^j E_j^a. \end{aligned} \quad (113)$$

Taking account of Eqs.(106)-(113), we obtain

$$\begin{aligned} \{H(N), H(M)\} &= \\ & \int_{\Sigma} (N D_c D^c M - M D_c D^c N) (-\tilde{K}_a^j E_j^a) \\ & + (N D^a M - M D^a N) (\pi D_a \phi) \\ & + (N D_a D^b M - M D_a D^b N) \tilde{K}_b^j E_j^a \\ &= \int_{\Sigma} (N D^a M - M D^a N) (D_a (\tilde{K}_c^j E_j^c) - D_b (\tilde{K}_a^j E_j^b) + \pi D_a \phi) \\ & - ((D_a M) D^b N - (D^b M) D_a N) \tilde{K}_b^j E_j^a \\ &= \int_{\Sigma} (N D^a M - M D^a N) V_a - \frac{[E^a D_a N, E^b D_b M]^i}{h} \mathcal{G}_i \end{aligned} \quad (114)$$

where we used the following identity

$$\begin{aligned} & -((D_a M) D^b N - (D^b M) D_a N) \tilde{K}_b^j E_j^a \\ &= -((D_a M) D_c N - (D_c M) D_a N) h^{bc} E_j^a \tilde{K}_b^j \\ &= -2(D_{[a} M)(D_{c]} N) \frac{E_i^b E_i^c}{h} E_j^a \tilde{K}_b^j \\ &= -2(D_a M)(D_c N) \frac{E_j^{[a} E_i^{c]}}{h} \tilde{K}_b^j E^{ib} \\ &= -\epsilon^{ijk} (D_a M)(D_c N) \frac{E_j^a E_i^c}{h} \tilde{K}_b^m E^{nb} \epsilon_{kmn} \\ &= -\frac{[E^a D_a N, E^b D_b M]^k}{h} \mathcal{G}_k. \end{aligned} \quad (115)$$

Using above result and shift conjugate pair (\tilde{K}_a^i, E_j^b) to (A_a^i, E_j^b) , we can easily get the Poisson bracket (46) between the smeared Hamiltonian constraints.

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